

## High-resolution optical spectroscopy investigation of Nd<sub>2</sub>BaNiO<sub>5</sub> and Nd<sub>0.1</sub>Y<sub>1.9</sub>BaNiO<sub>5</sub> and crystal-field parameters for rare-earth linear-chain nickelates

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### Abstract

High-resolution spectroscopy of Nd<sup>3+</sup> in Nd<sub>2</sub>BaNiO<sub>5</sub> and Y<sub>2</sub>BaNiO<sub>5</sub>:Nd(5%) powder samples is used to study Nd<sup>3+</sup> crystal-field levels and exchange splittings in these quasi-one-dimensional model compounds. We demonstrate that the Nd<sup>3+</sup> ground-state splitting in the magnetically ordered state of Nd<sub>2</sub>BaNiO<sub>5</sub> ( $T_N = 47.5 \pm 1$  K, as found from our spectroscopic data) accounts for the low-temperature magnetic properties and for the 4-meV mode observed earlier in inelastic neutron scattering experiments. Crystal-field analysis is performed. Its results show that the directions of ordered magnetic moments in Nd<sub>2</sub>BaNiO<sub>5</sub> are determined by the single-ion anisotropy of Nd<sup>3+</sup>. We argue that the crystal-field parameters obtained for Nd-nickelate (in this work) and Er-nickelate (in our earlier work) can be used to predict the energy-level patterns and magnetic properties of other rare-earth linear-chain nickelates. ©2005 The American Physical Society.

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